ELASTIC SCATTERING OF ELECTRONS BY HELIUM ATOM

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ABSTRACT. The S-wave phase-shifts (η_0) in the elastic $\bar{e}$-He collision problem have been computed by Hulthén's variational method in the energy range of 5 ev to 54.4 ev. The total wave function of the helium atom and electron system has been expanded in such a way as to include virtual excitation to $2\,^1S$ and $2\,^3S$ states. Our results for S-wave partial cross-sections have been compared with the theoretical findings of Marriott (1963), LaBahn and Callaway (1964), Moiseiwitsch (1953), and Zhikhareva (1965) and with the experimental results of Golden and Bandel (1965) and Ramsauer and Kollath (1929, 1932).

INTRODUCTION

The exchange and polarisation effects play important role in the scattering of electrons by atoms. These effects are especially important in the low-energy region. Marriott (1963) has employed a numerical method for the calculation of all significant partial cross-sections for elastic and inelastic collisions of electrons with helium atom. Explicit allowance has been made by him for electron exchange and all coupling terms between 1^1S, 2^1S and 2^3S states have been retained. LaBahn and Callaway (1964) have taken a complete antisymmetrized wave function to include exchange effect. Further, the formalism used by them was obtained from an extension of Hartree-Fock theory where the atomic distortion is approximated by a polarization potential. They have computed cross-sections for elastic scattering of electrons from helium atoms and have also given a tabulated values of partial wave phase shifts in the energy range of 0 to 54.4 ev. Zhikhareva (1965) has calculated the cross-sections for S-wave elastic scattering in $\bar{e}$-He collision assuming coupling of the 1^1S, 2^1S and 2^3S states of the helium atom. He has found two resonances (9.52 ev and 16.9ev) in the S-wave cross-section of elastic scattering of electron by helium atom.

In our previous work (1966) we have investigated the problem of $\bar{e}$-He collision, taking into consideration the virtual excitation to 2^1S state only, but neglecting the exchange effect. In the present work, however, we have considered the exchange effect and have also made allowance for the distortion induced in the atom by the scattering electron in the form of the virtual excitations to 2^1S and 2^3S

states in addition to the original ground state (1^1S). The virtual excitation to 2^1S and 2^3S states includes the coupling between the 1^1S, 2^1S and 2^3S states. Following Geltman (1965), we have formulated the problem such that the virtual excitation vanishes at the scattering centre and in the asymptotic region.

We have carried out calculations for S-wave phase-shifts by Hulthén's variational method in the energy range of 5 ev to 54.4 ev. Numerical computations have been performed by taking very small intervals in the energy region of 19 ev to 30 ev so as to get any resonance level in that region. Experiments by Schulz (1963), Simpson and Fano (1963), Kuyatt *et al* (1965) have indicated resonance level at 19.3 ev in the said energy region. Investigations have also been carried out with a wide energy interval in the rest of the energy region of 30 ev to 54.4 ev. The calculated values of S-wave elastic cross-sections have been compared with the theoretical results or Marriott (1963), LaBahn and Callaway (1964), Moiseiwitsch (1953) and Zhikhareva (1965). The experimental findings of Ramsauer and Kollath (1929, 1932) and Golden and Bandel (1965) have also been shown for comparison.

THEORY

The Schrödinger wave-equation for the electron and helium atom system is

$$(H-E)\psi(r_1, r_2, r_3) = 0 \qquad \ldots (1)$$

with $$H = -\frac{\hbar^2}{2m}(\Delta_1^2+\Delta_2^2+\Delta_3^2)-2e^2\left(\frac{1}{r_1}+\frac{1}{r_2}+\frac{1}{r_3}\right)$$

$$+e^2\left(\frac{1}{r_{12}}+\frac{1}{r_{13}}+\frac{e^2}{r_{23}}\right);\ E, \text{ the total}$$

energy of the system is given by $E = \frac{\hbar^2k^2}{2m} + E_0$ where E_0 = ground state energy of the helium atom and k = wave-number of the scattered electron, other symbols have their usual meanings. The co-ordinate wave function of the helium atom and electron system, considering the $1^1S-2^1S-2^3S$ states of the atom, may be written in the form (cf. Drukarev, 1965)

$$\psi(r_1,r_2, r_3) =$$

$$\frac{1}{\sqrt{2}}[\psi_1{}^1s\,(r_1, r_2,)\,F_1(r_3)-\psi_1{}^1(r_1, r_3)\,F_1(r_2)]$$

$$+\frac{1}{\sqrt{6}}[\psi_2{}^1s(r_1, r_2)F_2(r_3)-\psi_2{}^3S(r_1, r_3)\,F_2(r_2)+2\psi_2{}^3{}_s(r_3, r_2)\,F_2(r_1)]$$

$$+\frac{1}{\sqrt{2}}[\psi_2{}^1s(r_1, r_3)\,F_3(r_3)-\psi_2{}^1s(r_1, r_3)\,F_3(r_2) \qquad \ldots (2)$$

For the singlet state (1^1S) we take the Hylleraas (1929) wave function $\psi_1{}^1s(r_1, r_2) = \left(\frac{Z^3}{\pi}\right) e^{-Z(r_1+r_2)}$ where $Z = \frac{27}{16}$. We have used 2^1S wave function as given by Marriott and Seaton (1957) and 2^3S state wave function by Morse *et al.* (1935). These wave functions are as follow :

$$\psi_{2^1s}(r_1, r_2) = \frac{.478 \times 2^{1/4}}{\pi}\left\{\begin{matrix} e^{-2r_1}(e^{-1.136r_2} - .317\gamma_2 e^{-.446r_2}) \\ + e^{-2_2r}(e^{-1.136r_1} - .317r_1\, e^{-.464r_1}) \end{matrix}\right\}$$

$$\psi_{2^3s}(r_1, r_2) = = \frac{.882 \times 2^{1/4}}{\pi}\left\{\begin{matrix} e^{-2r_1}(e^{-1.57r_2} - .34r_2\, e^{-.61r_2}) \\ - e^{-2r_2}(e^{-1.57r_1} - .34r_1 e^{-.61r_1}) \end{matrix}\right\}$$

The functions $F(r)$ describe the state of the scattered electron. To take into consideration the virtual excitation of the atom to 2^1S and 2^3S states, we approximate the wave function of the total system of the electron and helium atom in the following form :

$$\psi(r_1, r_2, r_3) = \frac{1}{\sqrt{2}}\left[\psi_1{}^1s(r_1, r_2)\, F_0(r_3) - \psi_1{}^1s(r_1, r_3)\, F_0(r_2)\right]$$

$$+ \frac{1}{\sqrt{2}}\left[\psi_1{}^1s(r_1, r_2)\, F_1(r_3) - \psi_1{}^1s(r_1, r_3)\, F_1(r_2)\right]$$

$$+ \frac{1}{\sqrt{6}}\left[\psi_2{}^3s(r_1, r_2)\, F_2(r_3) - \psi_2{}^3s(r_1, r_3)\, F_2(r_2) + 2\psi_2{}^3s(r_3, r_2)\, F_2(r_1)\right]$$

$$+ \frac{1}{\sqrt{2}}\left[\psi_{2,5}(r_1 r_2) F_3(r_3) - \psi_{2,5}(r_1, r_3)\, F_3(r_2)\right] \qquad \ldots (3)$$

where $$F_0(r) = \frac{\sin kr}{kr} + a(1 - e^{-zr})\frac{\cos kr}{k\,r}$$

$$F_1(r) = (c_1 r + c_2 r^2)e^{-zr}$$

$$F_2(r) = (c_3 r + c_4 r^2)e^{-zr}$$

$$F_3(r) = (c_5 r + c_6 r^2)e^{-zr}$$

Here 'a' is the usual phase parameter $\tan \eta_0$ whereas, c_i ($i = 1, \ldots, 6$) are adjustable variational parameters.

To calculate η_0 by Hulthén's variational method, we define the variational integral in the usual way as $L = \int \psi^*(H - E)\psi dr_1 dr_2 dr_3$ and impose the condition.

$$L(a, c_i) = 0; \quad (i = 1, \ldots, 6) \qquad \ldots (4)$$

$$\frac{\partial L}{\partial c_i} = 0; \quad (i = 1, \ldots, 6) \qquad \ldots (5)$$

The co-efficients of c_i are evaluated for a particular energy. The six variables $c_i (i = 1, \ldots, 6)$ appearing in the six linear equations (5) are evaluated in terms of a by the method of matrix inversion for a particular energy. Substituting these values in (4), we get a quadratic equation in 'a' which yields the phase shift for the particular energy. The S-wave partial cross-section is then calculated by the formula $Q_{00} = \frac{4\pi}{k^2} \sin^2 \eta_0$.

RESULTS AND DISCUSSIONS

In the following table we have given our calculated S-wave partial cross-sections in the energy range of 20.606 ev to 27.365 ev. and have compared with the corresponding results of Marriott (1963). Our results compare favourably with those of Marriott (1963).

TABLE 1

Energy	S-wave cross-section R. Marriott	S-wave cross-section Present calculation
20.606	2.62	2.64
21.010	2.57	2.58
21.400	2.49	2.54
21.790	2.47	2.51
24.580	2.19	2.28
27.365	1.97	2.05

In fig. 1, the calculated values of scattering cross-sections have been plotted against energy and have been compared with theoretical results of Moiseiwitsch (1953), Zhikhareva (1965). The experimental findings of Ramsauer and Kollath (1929, 1932) have been shown for comparison. In fig. 2, we have plotted our calculated values of S-wave cross-sections against energy. A comparison has been made with the theoretical S-wave cross-sections calculated from the tabulated S-wave phase-shift values given by LaBahn and Callaway (1964), and experimental data of Golden and Bandel (1965). Perhaps a better choice of trial wave functions

containing a large number of adjustable linear as well as non-linear variational parameters might have led to the occurrence of resonance level in the energy region we have investigated.

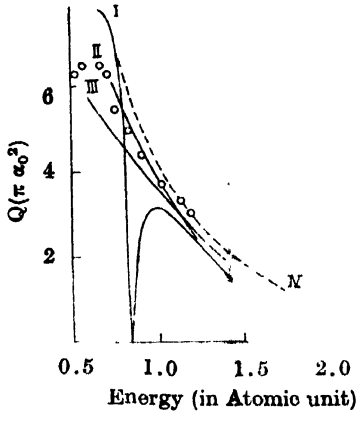

Fig. 1. The S-wave cross-section (in πa^2_0) plotted against energy (in atomic units) of the incident electron.

Curve I	Curve obtained from Zhikhareva (1965)
Curve II	Curve for broken bonds obtained from Zhikhareva (1965)
Curve III	Curve from calculations of Moiseiwitsch (1953)
Curve IV	Present calculations.
Circle	Experimental values of Ramsauer *et al*, (1929, 1932)

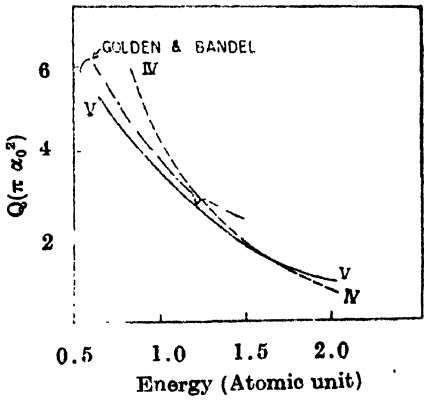

Fig. 2. The S-wave cross-section (in πa^2_0) plotted against energy (in atomic units) of the incident electron.

Curve IV Present calculations.

Curve V Cross section obtained from the tabulated S-wave phase shift values given by LaBahn *et al*, (1964).

— · — · Experimental curve of Golden *et al* (1965).

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